I. General Information

CAS Number: 2B Acid (CAS NO.: 88-51-7)
Name: 6-Amino-4-chloro-m-toluenesulfonic acid

CAS Number: C Amine or "C Acid"(CAS NO.88-53-9)
Name: 2-Amino-5-chloro-p-toluenesulfonic acid

II. Physical-Chemical Data

A1. Melting Point

Test Substance

Test substance: 6-Amino-4-chloro-m-toluenesulfonic acid

Remarks:

Method

Method: Measured
Remarks:

Results

Melting point value: 330 °C
Remarks:

References Company supplied data

Other

Data is consistent with melting points for the class of pigments and other available measurements

A2. Melting Point

Test Substance

Test substance:	2-Amino-5-chloro-p-toluenesulfonic acid
Remarks:	

Method

Method:	Estimated
Remarks:	

Results

Melting point value:	283.5 °C estimate, Adapted Joback method
Remarks:	

References

MPBPWIN v. 1.41 in EPIWIN v 3.10, Syracuse Research Corporation, Syracuse, New York

Other

Data is consistent with melting points for the class of compounds and other available measurements.

B. Boiling Point

Test Substance

Test substance: SOLID
Remarks:

Method

Method:
Remarks:

Results

Boiling point value:
Remarks:

References

Other

C1. Vapor Pressure

Test Substance

Test substance: 2-Amino-5-chloro-p-toluenesulfonic acid and 6-Amino-4-chloro-m-toluenesulfonic acid
Remarks:

Method

Method: Estimation
Remarks: Modified Grain method

Results

Vapor pressure value: 1.55E -008
Temperature:

Remarks:

References

MPBPWIN v1.40 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York

Other

C2. Vapor Pressure

Test Substance

Test substance: 4-Amino-m-toluenesulfonic acid
Tokyo Kasei Kogyo Co., Ltd.; purity 99.9%

Remarks:

Method

Method: Measured Value
Remarks: 1999

Results

Vapor pressure value: <.00052Pa
Temperature: 100 °C

Remarks:

References

Chemical Inspection and Testing Institute, Japan (1999): report on physical and chemical properties

Other

D. Partition Coefficient

Test Substance

Test substance: 4-Amino-m-toluenesulfonic acid

Remarks:

Method

Method: OECD TG107 (flask-shaking, no buffer used)
Remarks: 1999, GLP

Results

Log P_{OW}: -.67 at 25 °C
Remarks: sample weight: 1.06mg (= 5mL x 212mg/L)
component of test solution:
condition
case -1 mL -2 mL -3 mL

1-octanol saturated by water 5 10 20
water saturated by 1-octanol 30 25 15
---
temperature: 25(24-26)℃
revolution: 20/min x 5min
number of replicate: 2
analysis: HPLC

References

Chemical Inspection and Testing Institute, Japan (1999): report on partition coefficient between 1-Octanol and water

Other

E. Water Solubility

Test Substance

Test substance: 4-Amino-m-toluenesulfonic acid

Remarks: purity >99%

Method

Method: Measured Value 6 g/L at 20℃ **pH value :** = 3.8
Remarks:

Results

Value: 6.0 g/L
Temperature: 20 °C
Description: Soluble (1000-10000 mg/L)
Remarks:

References

Mitsuboshi Chemical Co., Ltd.: unpublished report

III. Environmental Fate Endpoints

A. Photodegradation

Test Substance

Test substance:	2-Amino-5-chloro-p-toluenesulfonic acid and 6-Amino-4-chloro-m-toluenesulfonic acid
Remarks:	

Method

Method:	Estimate
Test type:	Water\sunlight
Remarks:	

Results

Temperature:	
Degradation Rate	
: Half-life	
Ozone reaction:	7.20 hours, .6 days (12 Hour day; 1.5 E 6 OH/cm3)
Remarks:	n\a

Conclusions

References

AopWin v1.90 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York, SIDS DOSSIER 4B Acid

Other

A2. Photodegradation

Test substance:	4-Amino-m-toluenesulfonic acid
Remarks:	

Method

Method:	
Test type:	Estimation
Remarks:	Water

Results

Temperature:	
Hydroxyl radicals reaction	
OH Rate constant:	
Half-life	
Ozone reaction:	.4 days
Remarks:	

Conclusions

References

AopWin v1.90 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York, SIDS DOSSIER 4B Acid

Other

B. Stability in Water

Test Substance

Test substance:	4-Amino-m-toluenesulfonic acid
Remarks:	

Method

Method:	OECD Test 111 **t1/2 pH4 :** > 5 day(s) at 50℃ **t1/2 pH7 :** > 5 day(s) at 50℃ **t1/2 pH9 :** > 5 day(s) at 50℃
Test type:	abiotic hydrolysis
GLP:	no
Remarks:	1999

Results

Half-life:	pH 4 >5 days, pH 7 >5 days and pH 9 >5
Percent hydrolyzed in 5 days (120 hs) at 50 °C :	
Remarks:	

Conclusions The test substance has no activity of hydrolysis and is stable at pH 4, pH 7 and pH 9.

Data Quality

Remarks:

References Chemical Inspection and Testing Institute, Japan (1999): report on physical and chemical properties

C. Biodegradation

Test Substance

Test substance:	4-Amino-m-toluenesulfonic acid
Remarks:	purity >99%

Method

Method:	OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Test type:	Biological Oxygen Demand (BOD)
GLP:	no
Year:	1975
Remarks:	Degree of degradation after 28 days (Japanese standard activated sludge) **Control substance :** Aniline

Results

	Kinetic : 7 day(s) > 40 %
Results:	14 day(s) > 60 %
Remarks:	

Conclusions not biodegradable

Data Quality

Remarks:	under test conditions no biodegradation observed

References This was a well-documented study that followed established guidelines.

Other Chemical Inspection and Testing Institute, Japan (1999): report on biodegradation, Company supplied data.

D. Transport between Environmental Compartments (Fugacity)

Test Substance

Test substance: 2-Amino-5-chloro-p-toluenesulfonic acid and 6-Amino-4-chloro-m-toluenesulfonic acid

Remarks:

Method

Test type: Estimation

Model used: Level III Fugacity Model; EPIWIN:EQC from Syracuse Research Corporation

Remarks:

Results

Model data and results:

Distribution (%)	
Air	4.48 E-005
Water	46.4
Soil	53.5
Sediment	0.0755

Remarks: Since no experimental values were available the physical chemical values utilized in this model were default parameters from within EPIWIN.

Conclusions

References

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210. The Level III model incorporated in EPIWIN is a Syracuse Research Corporation adaptation of the methodology described by Mackay *et al.* 1996; *Environ. Toxicol. Chem.* **15(9)**, 1618-1626 and 1627-1637.

Other

IV. Ecotoxicity

A. Acute Toxicity to Fish

Test Substance

Test substance:	4-Amino-m-toluenesulfonic acid
Remarks:	Purity >95%

Method

Method:	OECD 203
Test type:	Flow through
GLP:	yes
Year:	1999
Species/strain:	Oryzias latipes (Orange Killifish)
Analytical monitoring:	yes; Exposure solutions, temperature, pH, dissolved oxygen
Exposure period:	96-Hour
Remarks:	A group of 10 fishes were exposed to 10 mg/L, Solvent Control (.<.1mg/l) and laboratory water control

Results

Nominal concentration:	
Measured concentration:	
Endpoint value:	96-hour LC_{50} >10 mg/L
Biological observations:	
Statistical methods:	
Remarks:	

Conclusions NO abnormal behavior, abnormal respiration nor dad were observed in any dose level

Data Quality

Reliability:	Reliable without restrictions
Remarks:	

References Report No. EFA98002, Environment Agency, Japan (1999a): unpublished report

Other

A2. Acute Toxicity to Fish

Test Substance

Test substance:	2-Amino-5-chloro-p-toluenesulfonic acid and 6-Amino-4-chloro-m-toluenesulfonic acid
Remarks:	

Method

Method:	Estimation
Test type:	
GLP:	
Year:	2006
Species/strain:	fish
Analytical monitoring:	
Exposure period:	
Remarks:	

Results

Nominal concentration:	
Measured concentration:	
Endpoint value:	96 Hour LC 50 91074.4 mg/L
Biological observations:	
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	
Remarks:	

References

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210.

Other

The ECOSAR model incorporated in EPIWIN is a Syracuse Research Corporation adaptation of the methodology described by Mackay *et al.* 1996; *Environ. Toxicol. Chem.* **15(9)**, 1618-1626 and 1627-1637.

B. Acute Toxicity to Aquatic InvertebratesTest Substance

Test substance: 4-Amino-m-toluenesulfonic acid
Purity >95%

Remarks:

Method

Method:
Test type: OECD 202.
GLP: Static
Year: Yes
Species/strain: 1999
Analytical monitoring: Daphnid (*Daphnia magna*)
Exposure period: No
Remarks: 48 hours

Results

Nominal concentration:
Measured concentration: 10 mg/L
Endpoint value:

48 -hour LC_{50}>10mg/l,

Reproduction

Biological observations:

Statistical methods:

Remarks: 5 daphnids (4 replicates; 5 organisms per replicate) were exposed to 1 nominal concentrations (10 mg/L) control of DMSO: HCO-40 =9:1 (100mg/L) and laboratory water control

Conclusions

Data Quality

Reliability: Reliable without restrictions
Remarks: This was a well-documented OECD guideline study conducted under GLP assurances.

References

Report No. EDI98002, Environment Agency, Japan (1999b): unpublished report
EA Japan (1999) OECD SIDS DOSSIER 4B ACID
Data for Chronic Toxicity to aquatic invertebrates also available

Other

C. Toxicity to Aquatic Plants

Test Substance

Test substance:	4-Amino-m-toluenesulfonic acid Purity >95%
Remarks:	

Method

Method:	OECD 201
Test type:	Biomass
GLP:	Yes
Year:	1999
Species/strain:	Selenastrum capricornutum
Endpoint basis:	
Exposure period:	72 hours
Analytical procedures:	Yes
Remarks:	

Results

Nominal concentration:	10/mg/L
Measured concentration:	
Endpoint value:	EC_{50} >10mg/L
NOEC:	>10 mg/L
Biological observations:	
Was control response satisfactory:	Yes
Statistical Methods:	
Remarks:	

Conclusions No growth inhibition was observed to green algae up to 10 mg/L

Data Quality

Reliability:	reliable with restriction
Remarks:	

References Report No. EDR98002, Environment Agency, Japan (1999c): unpublished report. EA Japan (1999) OECD SIDS DOSSIER 4B ACID

Other

V. Toxicological Data

A. Acute Toxicity

Test Substance

Test substance:	2-Amino-5-chloro-p-toluenesulfonic acid and 6-Amino-4-chloro-m-toluenesulfonic acid
Remarks:	Purity was unknown

Method

Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	No (Pre-GLP)
Year:	1968
Species/strain:	Rat/unknown
Route of exposure:	Oral gavage
Dose levels:	Unknown
Remarks:	

Results

Value:	LD_{50} = >7,500 mg/kg 2B acid
Deaths at each dose:	
Remarks:	

Conclusions Material would be considered as not toxic.

Data Quality

Reliability:	Reliable with restrictions
Remarks:	

References

Other

Acute toxicity

Test substance:	4-Amino-m-toluenesulfonic acid 99%Purity
Remarks:	

Method

Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	Yes
Year:	1996
Species/strain:	Rat
Route of exposure:	Oral gavage
Dose levels:	0,100,250,500,1000,2000 mg/kg/day
Remarks:	

Results

Value:	LD_{50} = >2,000 mg/kg.
Deaths at each dose:	
Remarks:	

Conclusions Material would be considered as not toxic.

Data Quality

Reliability:	Reliable without restrictions
Remarks:	

References

Ministry of Health & Welfare, Japan (1996a): Toxicity Testing Reports of Environmental Chemicals, vol.4 p. 99-106, "Twenty-eight-day Repeat Dose Oral Toxicity Test of 2-Amino-5- methylbenzenesulfonic acid in Rats".

Other

Repeated Dose Toxicity Test

Substance

Test substance:	4-Amino-m-toluenesulfonic acid
Remarks:	Commercial purity 98%

Method

Method:	OECD 407
Test type:	Repeat Dose
GLP:	Yes
Year:	1996
Species/strain:	Rat Male and Female
Route of exposure:	Gavage
Duration of test:	42 days
Exposure levels:	0. 100, 300 or 1,000 mg/kg
Sex:	Male and female
Exposure period:	28 days
Post-exposure observation period:	
Remarks:	

Results

NOAEL (NOEL): 300 mg/kg/day

No change in mortality and behavior were observed in any groups.
body weight and food consumption: No toxic effect was observed in any groups. urinary findings: Increase of specific gravity and decrease of pH were observed in 1000 mg/kg males. However no related change was observed in other findings. hematological findings: Slight decrease of white blood cell count (due lymphopenia) were observed in 1000 mg/kg males. No pathological change was observed in the lymphatic tissues, such as marrowcyte, thymus, lymphknote and spleen. blood chemical finding: Slight increase of GPT in females, slight decrease of total cholesterol in males and slight decrease of glucose in females were observed in 1000 mg/kg group. However, including liver, no pathological change was observed in any of related organs. According to the author, the change is within normal range, based on their other study data. necropsy finding: Slight enlargement of cecum was observed in one male and one female in 1000 mg/kg group. However no diarrhea and no growth abnormalities were observed. weight of organs: Decrease of thymus weight in 100 mg/kg and increase of spleen weight in all dose levels in female were observed. However those changes were no relation with dose levels.
remark: All of above changes returned to normal during 14 days recovery period.

Conclusions Test substance is not significantly toxic

Data Quality

Reliability: Reliable without restriction Remarks:

References: Ministry of Health & Welfare, Japan (1996a): Toxicity Testing Reports of Environmental Chemicals, vol.4 pp. 99-106, "Twenty-eight-day Repeat Dose Oral Toxicity Test of 2-Amino-5-methylbenzenesulfonic acid in Rats".

C. **Genetic Toxicity - Mutation**

Test Substance

Test substances:	2-Amino-5-chloro-p-toluenesulfonic acid and 6-Amino-4-chloro-m-toluenesulfonic acid
Remarks:	

Method

Method:	In Vitro Mutagenicity
Test type:	Ames
GLP:	Unknown
Year:	1985 C Amine, 1988 2B Acid
Species/strain:	Salmonella typhimurium
Metabolic activation:	Yes
Concentration tested:	
Remarks:	

Results

Result:	Negative
Cytotoxic concentration:	
Precipitation concentration:	Negative
Genotoxic effects	Negative
With activation:	
Without activation:	
Statistical methods:	
Remarks:	

Conclusions Reliable with restrictions, studies are well documented.

Data Quality

Reliability:	Hidesuke Shimizu et al., JPN J. Ind. Health, Vol27, pp. 400-419 (1985) (C Amine), Yoshimi, N., Sugie, S., Iwata, H et al. Mutation Research Vol. 206, pp.183-191, 1988 (2B Acid)
Remarks:	

References

C. **Genetic Toxicity - Mutation**

Test substance: 4-Amino-m-toluenesulfonic acid Remarks: 98% pure

Method

Method: OECD 471, 472

Test type:	Ames
GLP:	Yes
Year:	Japan (1996)
Species/strain:	Salmonella typhimurium
Metabolic activation:	With and without
Concentration tested:	5000 ug/plate with and without activation
Remarks:	

Results

Result:	Negative in all bacterial strains with and without activation
Cytotoxic concentration:	
Precipitation concentration:	
Genotoxic effects	
With activation:	Negative
Without activation	Negative
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability: Reliable without restriction Remarks:

References Report No. CTL/P/1999, Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers, unpublished report.

Other

D. Genetic Toxicity – Chromosomal Aberrations

Test Substance

Test substance:	4-Amino-m-toluenesulfonic acid Commercial purity 99%
Remarks:	

Method

Method:	
Test type:	OECD 473
GLP:	Cytogenetics Assay
Year:	Yes
Species/strain:	1996
Exposure period:	Chinese Hamster CHL Cells
Remarks:	

Results

Result:	
Genotoxic effects:	Negative
Concentration tested	Negative
Statistical methods:	0, 16, 80, 400, or 2000 ug/mL
Remarks:	

Conclusions

This chemical induces weak chromosomal aberration to CHL/IU cell with an exogenous metabolic activation system. However, origin of the aberration is due to the acidity, but not due to physiological DNA damage.(The low acidity effect is reported in [T.Morita et al., Mutation Res, 268, 297 1992].)

Data Quality

Reliability:	
Remarks:	Reliable without restriction

References

Other

Ministry of Health & Welfare, Japan (1996c): Toxicity Testing Reports of Environmental Chemicals, vol.4 p111-114, "In Vitro Chromosomal Aberration Test of 2-Amino-5-methylbenzenesulfonic acid on Cultured Chinese Hamster Cells".

E. **Developmental Toxicity**

Test Substance Description included in OECD 422 study described above

Test substance:

Remarks:

Method

Method:

GLP:

Year:

Species/strain:

Sex:

Route of exposure:

Exposure levels:

Actual doses received:

Exposure period:

Duration of test:

Remarks:

Results

Maternal toxicity

NOEL:

NOEL for teratogenicity:

NOEL for fetotoxicity:

Parental toxic responses:

Fetal toxic responses dose:

Statistical Methods:

Remarks:

Conclusions

Data Quality

Reliability:

Remarks:

References

Other

F. Toxicity to Reproduction

Test Substance

Test substance:	2-Naphthalenecarboxylic acid, 3-hydroxy-4-[(4- methyl-2-sulfophenyl)azo]-, calcium salt
Remarks:	Commercial purity 98%

Method

Method:	OECD 421
GLP:	Yes
Year:	1999
Species/strain:	Rat
Sex:	male and female
Route of exposure:	gavage
Exposure levels:	0,100,300 or 1000 mg/kg
Exposure period:	males 48 days including /females 41-48 days
Duration of test:	
Remarks:	

Results

Maternal toxicity NOEL:	Parental, 1000 mg/kg/day
Parental toxic responses:	
Fetal toxic responses dose:	
Statistical Methods:	
Remarks:	No effects were observed in the copulation index, fertility index, gestation length, number of corpora lutea or implantations, implantation index, gestation index, parturition or maternal behavior. There were no significant differences in number of offspring or live offspring, sex ratio, the live birth index, the viability index and the body weight. No abnormal findings related to the test substance were noted for external features, clinical signs, or on necropsy finding for the offspring. No pups with malformation were found in any group. No change in clinical signs and necropsy finding were observed in offspring.

Conclusions

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References

Ministry of Health & Welfare, Japan (1999): Toxicity Testing Reports of Environmental Chemicals, vol.7 p163-171, "Preliminary Reproduction Toxicity Screening Test of 2-Amino-5-methylbenzenesulfonic acid by Oral Administration in Rats".

Other

Acute toxicity

Test substance: 2-Naphthalenecarboxylic acid, 3-hydroxy-4-(5-chloro-4- methyl-2-sulfophenyl)azo]-, Barium salt **and** 2-Naphthalenecarboxylic acid, 3-hydroxy-4-(5-chloro-4- methyl-2-sulfophenyl) azo]-, Calcium salt

Remarks:

Method

Method:	Irritation to the rabbit eye
Test type:	eye irritation
GLP:	unknown
Year:	1972
Species/strain:	rabbit
Route of exposure:	
Dose levels:	
Remarks:	

Results

Value:	negative
Deaths at each dose:	
Remarks:	

Conclusions

Data Quality

Reliability:	unassignable
Remarks:	

References **Company data**

Other

Acute toxicity

Test substance:	2-Naphthalenecarboxylic acid, 3-hydroxy-4-(5-chloro-4- methyl-2-sulfophenyl)azo]-, Barium salt **and** 2-Naphthalenecarboxylic acid, 3-hydroxy-4-(5-chloro-4- methyl-2-sulfophenyl)azo]-, Calcium salt
Remarks:	

Method

Method:	Skin irritation to the rabbit
Test type:	Skin irritation
GLP:	unknown
Year:	1972
Species/strain:	rabbit
Route of exposure:	
Dose levels:	
Remarks:	

Results

Value:	negative
Deaths at each dose:	
Remarks:	

Conclusions

Data Quality

Reliability:	unassignable
Remarks:	

References **Company data**

Other

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